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EXECUTIVE SUMMARY

A STRUCTURED SYSTEM FOR CALCULATION OF AIR PARCEL TRAJECTORIES

S.C. Wright
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Atmospheric Research Section

In 1981, as part of an effort to determine the impact of Ontario Hydro's acid gas emissions on sensitive receptors, a proposal for a long-range transport modelling program was submitted. Since the budgeted resources were not sufficient to undertake the full program, it was decided to implement the most useful component - the trajectory module. The objective was to use wind field data to calculate trajectories forward in time from Ontario Hydro's fossil-fuel fired generating stations and backward in time from acidic deposition monitoring samplers.

The geostrophic wind technique was selected based on a review of available ways to construct a wind field. The wind field is calculated by adjusting the geostrophic wind field, which is computed from surface pressure data, to account for surface frictional effects. Given this wind field, chronologically arranged trajectories either forward or backward in time are calculated.

The system of computer programs for trajectory calculation according to the method just described has been implemented on the UNIVAC mainframe computer. Components of the software package have been tested on the UNIVAC, but because of the prohibitive costs that would be involved in full-scale testing on the UNIVAC, the computer programs were transferred to the HP1000 minicomputer. Code revisions are necessary to have the software executable on the HP1000. Detailed documentation and final testing using several sets of real data are required to fully complete the trajectory software system. There are no immediate plans to proceed with this work.

job	file	date	report no.
740635-634-091	837.2212	January 4, 1985	84-357-K

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To Mr. F.J. Kee
Dirctor of Research

A STRUCTURED SYSTEM FOR
CALCULATION OF AIR PARCEL TRAJECTORIES

S.C. Wright

ABSTRACT

A structured system of computer programs for calculation of air parcel trajectories was developed with the objective of having a facility with which to calculate trajectories forward in time from Ontario Hydro's fossil-fuel fired generating stations (or other sources) and backward in time from samplers. The software was implemented and partially tested on the UNIVAC mainframe computer and then was transferred to the HP1000 minicomputer. Detailed program documentation, some code modifications and final testing using several sets of real data are necessary to complete the software package.

1.0 INTRODUCTION

The Atmospheric Research Section has been involved in an effort to determine the impact of Ontario Hydro's acid gas emissions on sensitive receptors. As part of this effort, a software package for calculation of air parcel trajectories has been developed and implemented. The objective in implementing this trajectory system was to have a facility with which to calculate trajectories forward in time from Ontario Hydro's generating stations and backward in time from acidic deposition monitoring samplers.

The system of computer programs for trajectory calculation was implemented on the UNIVAC mainframe computer and has been stored in both the onsite and offsite Atmospheric Research Section magnetic tape libraries. The software was also transferred to the Section's HP1000 minicomputer, but the package is not operational on this computer system.

job	file	date	report no.
740635-634-091	837.2212	January 4, 1985	84-357-K

This report describes the initial stages of the project, the approach followed, the status of the work and the requirements for full completion of the trajectory software system.

2.0 BACKGROUND

In 1981, a proposal for a modelling program to answer questions about long-range transport of atmospheric pollutants was submitted (Misra and Ryman, 1981). In this proposal the objectives of the model development were discussed, some theoretical background to the three model types (i) statistical; (ii) Lagrangian; (iii) Eulerian was given and the rationale for selecting and developing a Lagrangian model was provided. The specific theoretical form of the Lagrangian model was outlined along with the planned computer implementation with detailed time and cost estimates.

Eight modules were to be developed (Figure 1).

1) Data Assembly - acquire and organize historical meteorological and source emissions data,

2) Trajectory - use wind field data to calculate chronologically arranged trajectories, where each trajectory is a time sequence of spatial coordinates,

3) Statistics - compute mean position, standard deviation and correlation of trajectory coordinates as a function of travel time,

4) Transport - a complicated module which would compute the contribution to gas concentrations, and precipitation acidity of an emission source,

5) Graphics - display output from transport module,

6) Scenario - calculate total contributions from all sources,

7) Observation - interpolate observed receptor data onto model grid,

8) Verification - compare observations with model predictions.

Along with the model structure, the required model tasks were drawn up (Figure 2).

Several meetings of a potential study team were held. At this point it became apparent that the budgeted resources were not sufficient to undertake the full program. It was decided that the most useful system component from the long-range transport proposal to implement and study was the trajectory module.

LRT MODEL STRUCTURE

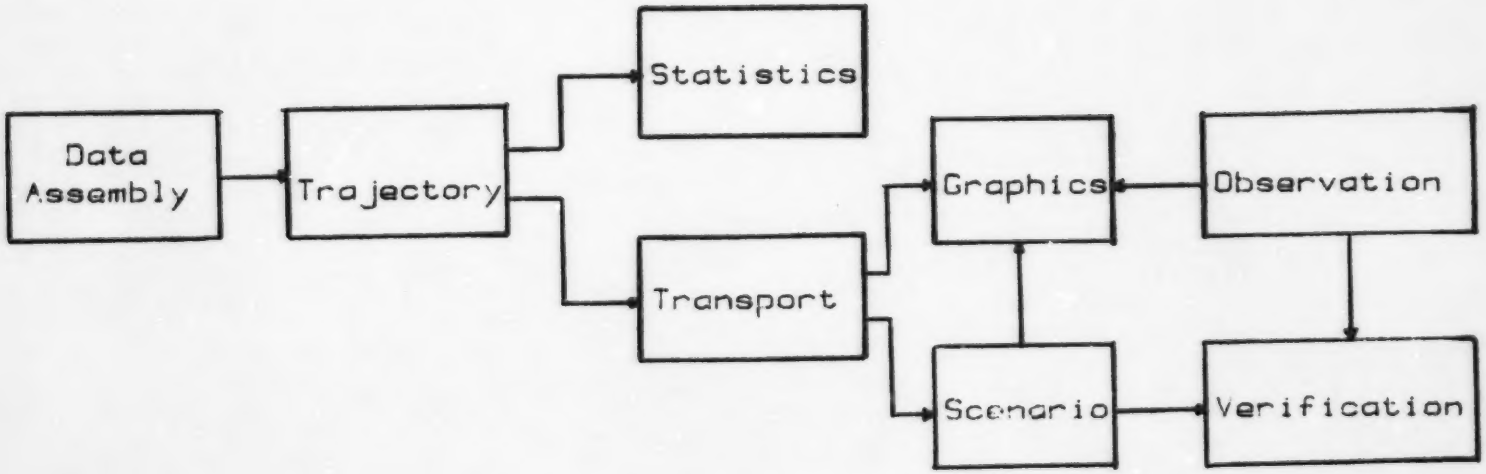


Figure 1

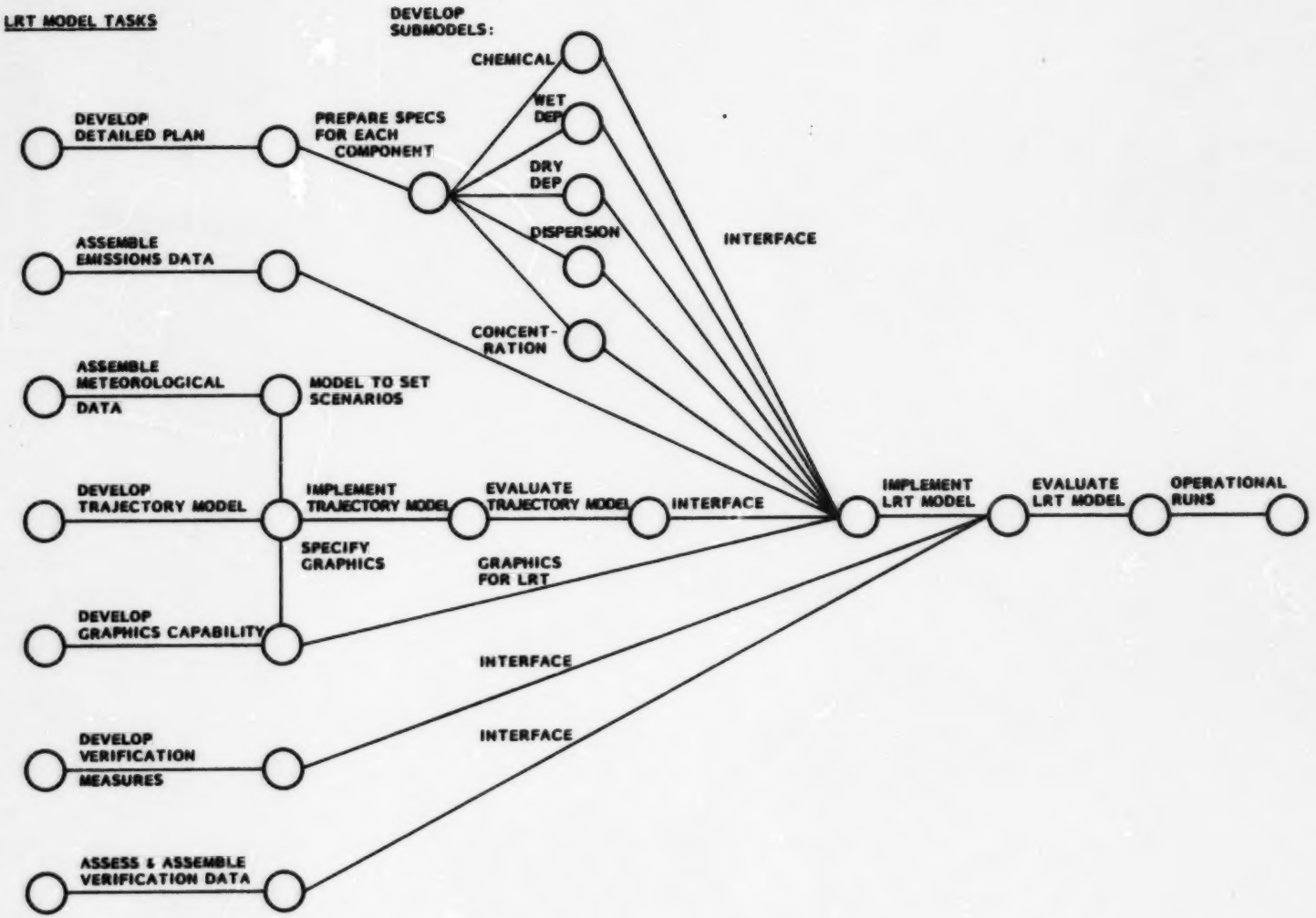

LRT MODEL TASKS
DEVELOP SUBMODELS:
CHEMICAL
WET DEP
DRY DEP
DISPERSION
CONCENT-RATION
DEVELOP DETAILED PLAN
PREPARE SPECS FOR EACH COMPONENT
ASSEMBLE EMISSIONS DATA
ASSEMBLE METEOROLOGICAL DATA
MODEL TO SET SCENARIOS
DEVELOP TRAJECTORY MODEL
IMPLEMENT TRAJECTORY MODEL
EVALUATE TRAJECTORY MODEL
INTERFACE
SPECIFY GRAPHICS
GRAPHICS FOR LRT
DEVELOP GRAPHICS CAPABILITY
INTERFACE
DEVELOP VERIFICATION MEASURES
INTERFACE
ASSESS & ASSEMBLE VERIFICATION DATA
INTERFACE
IMPLEMENT LRT MODEL
EVALUATE LRT MODEL
OPERATIONAL RUNS

FIGURE 2

3.0 TRAJECTORY CALCULATION METHOD

Trajectories are traditionally calculated as two-dimensional horizontal tracks, while the wind field from which they are derived is three-dimensional. The ideal situation would be to be able to construct a trajectory from the 'best' three-dimensional wind field. But the definition of the 'best' three-dimensional wind field is not well-defined. One way to construct a wind field is to use those meteorological data that are available. Two regular archived data sets that are available are:

- upper level data obtained by radiosonde every 12 hours at the network of radiosonde stations shown in Figure 3,

- surface data obtained by standard meteorological instrumentation every hour at the radiosonde and surface stations in Figure 3.

Using these two data sets there are four ways to construct a wind field. Using:

- surface wind data,
- upper level wind data,
- wind field analysis,
- surface pressure data.

Surface wind data are virtually never used since there are too many local topographical effects such as buildings, valley, lake/land interfaces, etc.

Measured upper level wind data would be the best to use to construct a wind field, but these data are sparse in space and time.

Fundamentally, wind field analysis is based on upper level wind, so the same problem with sparseness in space and time is encountered. Also, there is difficulty in archiving wind field analysis data.

Surface pressures are much less affected by local variations and so provide a smoother field of data. Surface pressure data can be used to obtain the geostrophic wind (Sykes and Hatton, 1976). A correction must be used to adjust the initial estimate of the wind away from the geostrophic wind. Such a correction accounts for surface frictional effects.

Based on this review of available techniques, it was decided to implement the goestrophic wind technique.

To calculate a geostrophic wind field from surface pressure data, it is required first to interpolate the surface pressures collected from the reporting stations onto a grid, then calculate the geostrophic wind field from the gridded pressures and finally integrate the wind field over time to obtain trajectories. The data flow diagram in Figure 4 illustrates the structure of the system which calculates air parcel trajectories using the geostrophic wind technique.

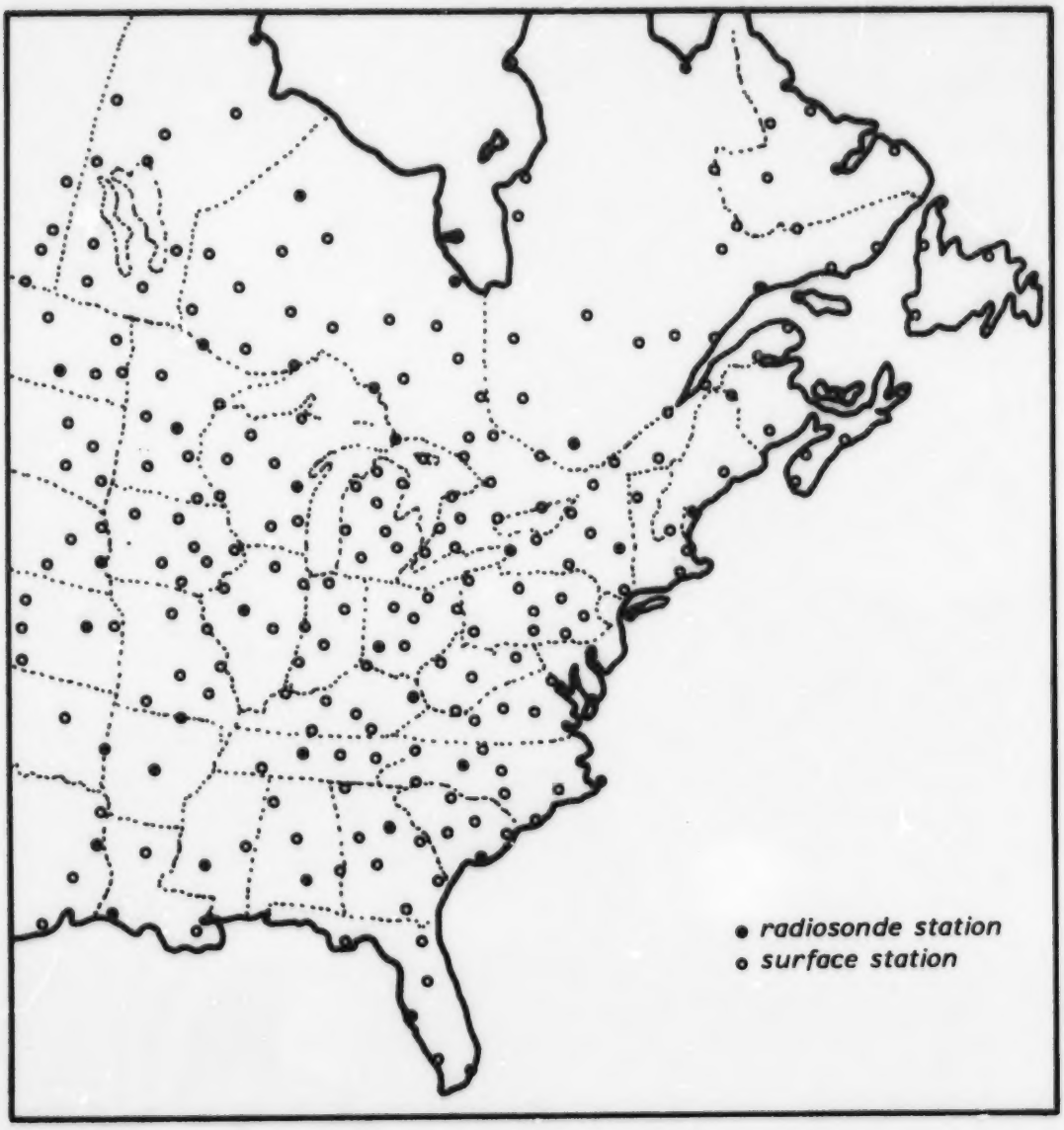


FIGURE 3
STATION NETWORK

167252 RD

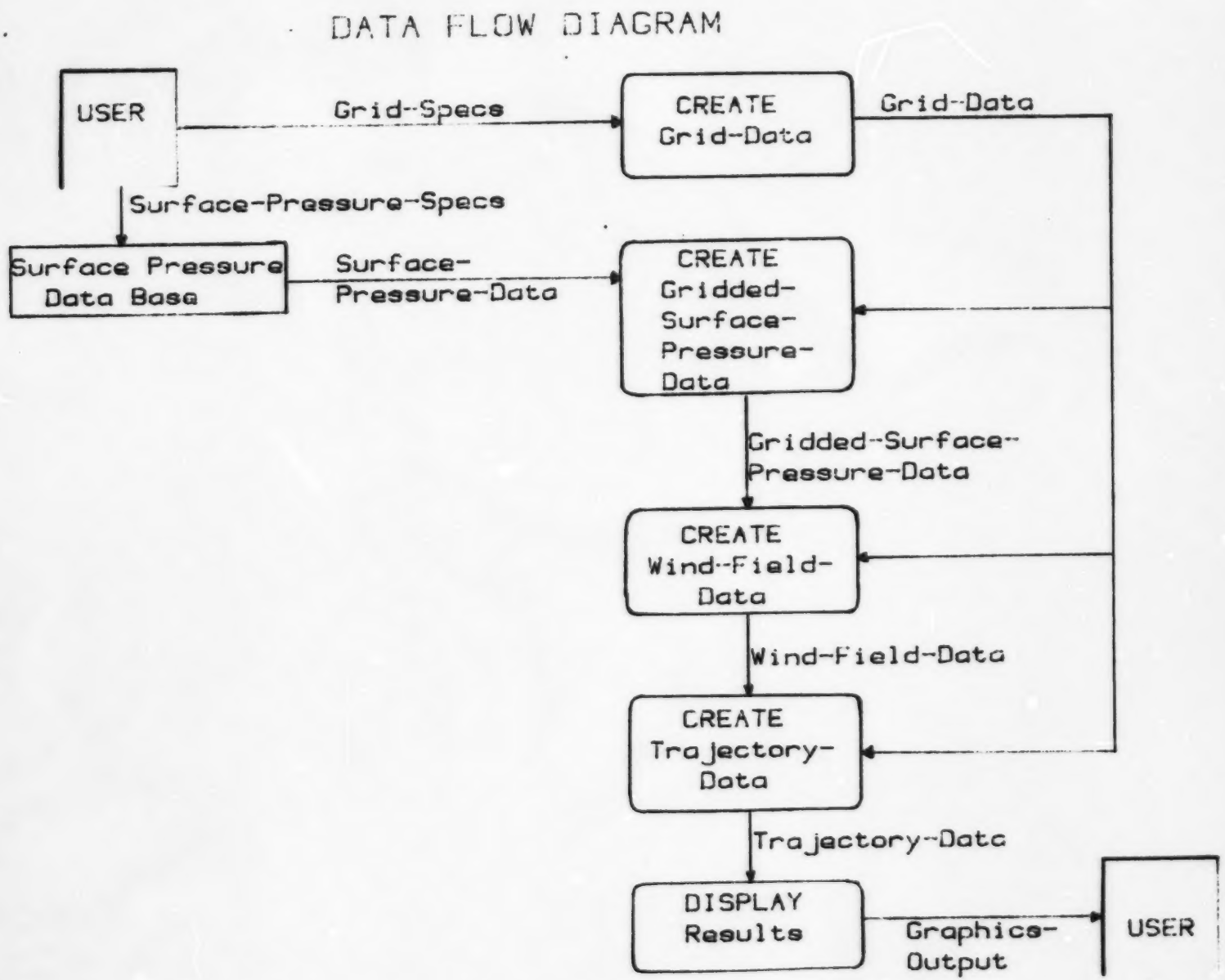

DATA FLOW DIAGRAM
USER
Grid--Specs
CREATE Grid-Data
Grid--Data
Surface-Pressure-Specs
Surface Pressure Data Base
Surface-Pressure-Data
CREATE Gridded-Surface-Pressure-Data
Gridded--Surface--Pressure-Data
CREATE Wind--Field-Data
Wind--Field-Data
CREATE Trajectory-Data
Trajectory--Data
DISPLAY Results
Graphics-Output
USER

Figure 4

3.1 Surface Pressure Data

A surface pressure data base has been established with the cooperation of the Resource Utilization Department (RUD) in the Power System Operation Division. Hourly surface pressure data from more than 365 weather stations in North America have been collected from September, 1981 to date from RUD. These data are stored in the Atmospheric Research Section's onsite magnetic tape library. Surface pressure data from September, 1980 through to September, 1981 are also available (Schaedlich, 1982).

3.2 Grid System

It was decided that input and output to the trajectory system should be independent of a particular grid system. For example, when inputting the location of a surface pressure reporting station, this would be given as a latitude and longitude rather than x and y coordinates of a grid. The final output of trajectories, given as a set of coordinates, would also be given as latitudes and longitudes.

However, before calculating the geostrophic wind from the surface pressures, it is necessary to obtain gridded surface pressure data by interpolating the surface pressures reported from the weather stations onto a grid. The following grid system is used.

Consider the earth as a sphere with radius equal to 6371.1 kilometers and the coordinate system x,y,z (Figure 5) such that:

- x is the axis through the equator and 0 degrees longitude
- y is the axis perpendicular to the x axis through 90 degree east longitude
- x is the axis perpendicular to the x and y axes through the north pole

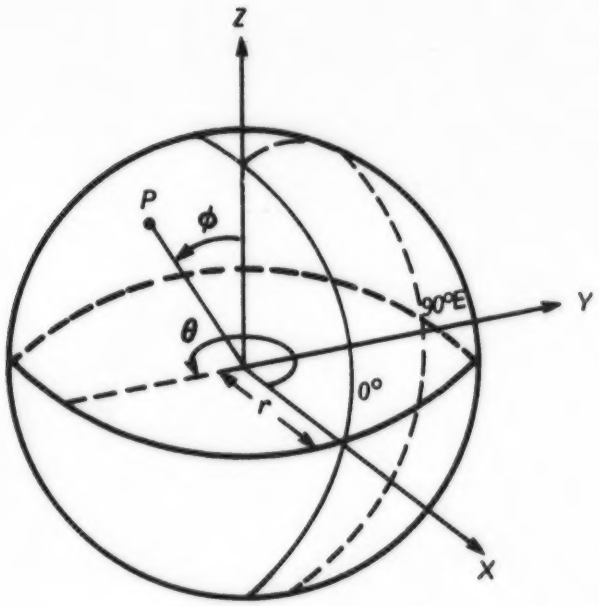
The origin (0,0,0) corresponds to the centre of the earth. θ is defined as (360 degrees - the longitude) when measured west and as the longitude alone when measured east. ϕ is defined as (90 degrees - the latitude) when measured north and as (90 degrees + the latitude) when measured south. A point P defined by θ and ϕ would have coordinates (p_1, p_2, p_3) in the (x,y,z) coordinate system where:

$$p_1 = r \cos \theta \sin \phi$$
$$p_2 = r \sin \theta \sin \phi$$
$$p_3 = r \cos \phi$$

Now consider a coordinate system defined by u,v and w (Figure 6) where:

- w is the axis passing through the centre of the earth and a specified point on the surface of the earth θ_c, ϕ_c called the grid orientation point

X, Y, Z Coordinate System



$r = 6371.1$ km

$P = (p_1, p_2, p_3)$

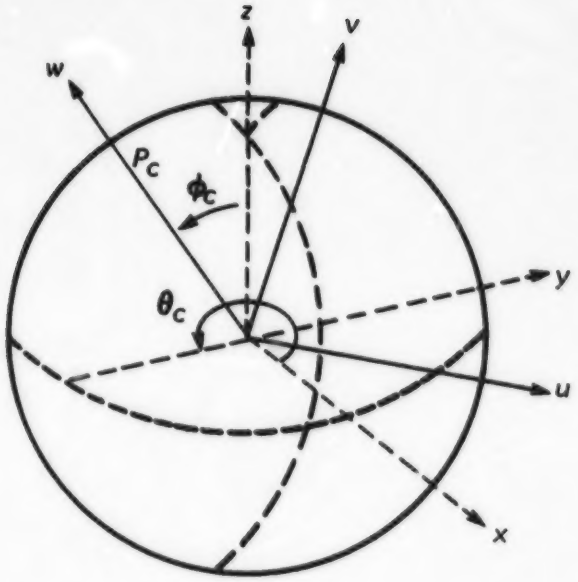
$p_1 = r \cos\theta \sin\phi$

$p_2 = r \sin\theta \sin\phi$

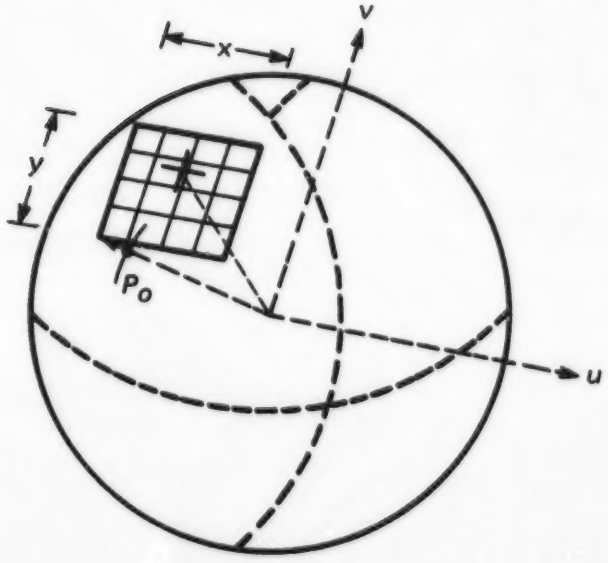
$p_3 = r \cos\phi$

FIGURE 5

u,v,w Coordinate System



P_C = (0, 0, 6371.1) *grid orientation point*



P_O - *point on the surface of the earth which defines the grid origin*
x,y - maximum x and y grid lengths

FIGURE 6

- v is perpendicular to u and parallel to the longitude given by ϕ_c

- u is perpendicular to v and w.

The point defined by θ_c and ϕ_c would have coordinates (0,0,6371.1) and the grid is defined as the u-v plane. A grid to cover an area of interest, say an area of northeastern North America, is selected by specifying the grid orientation point given by a latitude and longitude, the grid origin (the lower left-hand starting grid point given also by latitude and longitude), a grid unit length in kilometers and maximum x and y grid lengths (Figures 6,7). The points on the surface of the earth are then projected into this grid.

3.3 Gridded Surface Pressure Data

In calculating the surface pressures at each of the grid points, the orthogonal polynomial method is used (Marriott, 1981). The orthogonal polynomial method uses the principles of linear regression. The observations (in this case they are the surface pressure readings taken at each station) are considered to be a function of the data points (which are the station locations given as latitude and longitude). The form of the polynomial expression which represents this function is predetermined by a total degree and the number of components in the data points. There are two components, latitude and longitude, for this application. It is required to find the coefficients of the polynomial which will represent most exactly the observations, ie, the distance between the observations and the polynomial is minimized. For this application, it is required to approximate surface pressures by a polynomial with 10 terms. The polynomial is then used to approximate surface pressures at each of the grid points.

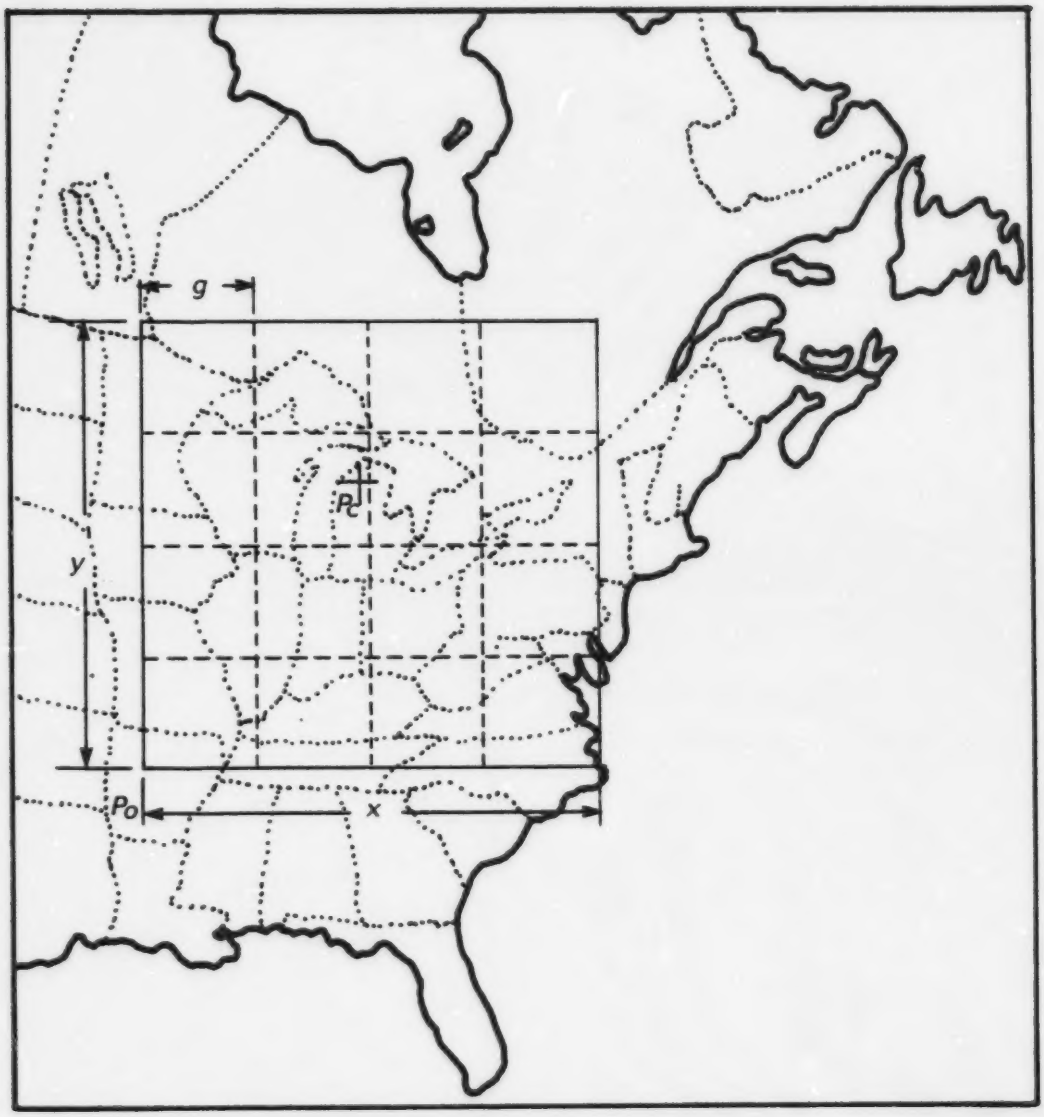
3.4 Wind Field

From the gridded surface pressures, a geostrophic wind field is calculated.

There are three major acting forces when considering the horizontal motion of air in the atmosphere (Byers, 1959):

- pressure gradient force
- Coriolis force
- frictional force

A parcel of air will experience a net force when there is a difference between the pressures on surfaces at opposite sides. This is called the pressure gradient force. Most large scale atmospheric motions in the middle latitudes are driven by the pressure gradient force.



P_c - grid orientation point = 45°N, 85°W

P_o - grid origin = 35°N, 93°W

x,y - maximum x,y grid lengths = 1524, 1524 km

g - grid unit length = 381 km

FIGURE 7

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Because of the rotation of the earth around its own axis, a force must be introduced in the equation of motion written in the coordinate system fixed to the earth's surface. This force is called the Coriolis force.

There exist considerable frictional forces between the atmosphere and the earth's surface.

In upper levels of the atmosphere where the frictional force is small, the Coriolis force is balanced principally by the pressure gradient. The air velocity determined by the balance of Coriolis and pressure gradient forces is called the geostrophic wind. For middle and high latitudes, the geostrophic wind is usually a good approximation to the observed wind velocity in the absence of frictional forces and is represented by:

$$\frac{1}{\rho}\frac{\partial p}{\partial x} = 2\Omega v \sin\phi$$

$$\frac{1}{\rho}\frac{\partial p}{\partial y} = -2\Omega u \sin\phi$$

where

u,v are the components of the geostrophic wind

ρ is the air density

$\frac{\partial p}{\partial x}, \frac{\partial p}{\partial y}$ are the components of the pressure change

Ω is the angular velocity of the earth

ϕ is the latitude

After computing, the geostrophic winds they must be modified in order to consider surface frictional effects. The following procedure (Chung, 1977) is applied:

$$V = k\, V_g$$

where:

$V(u,v)$ is the wind after adjustment of the geostrophic wind speed

k is the modification constant

$k = 0.42 + 0.04|r| + 0.024\, V_g$; $k = 0.9$ if $V_g \geq 16$ and $|r| \geq 3.1$

r is the 3-hourly pressure tendency

The final adjusted wind, V, is obtained from the following:

$$u_a = u\cos\sigma + v\sin\sigma$$

$$v_a = v\cos\sigma - u\sin\sigma$$

$\sigma = 50.3 - 2.7|r| - 1.8\, V$; $\sigma = 15$ if $V_g \geq 16$ and $|r| \geq 3.1$.

3.5 Trajectories

The trajectories are calculated using the final adjusted wind field. Given an initial location on the grid (which is given as latitude and longitude and then translated into grid coordinates), an initial time (starting date and time of the trajectory), a time interval (time step between trajectory position changes) and a maximum time (length of time between start and end of the trajectory), a sequence of trajectory positions (either forward or backward in time) is computed. A point is moved from a given starting position to its next position based on a weighted average of the wind speed and direction from the four surrounding grid points. The distance from the given position to each of the four surrounding points is calculated and weighting factors are computed based on these distances. Then the weighted average wind speed and direction is used to calculate the new position on the grid. This time sequence of grid coordinates is translated into corresponding latitudes and longitudes for final output.

4.0 Project Status and Requirements for Completion

A system of computer programs for the calculation of air parcel trajectories according to the method described in the preceding section has been developed and implemented on the UNIVAC mainframe computer. Figure 8 illustrates gridded surface pressures computed from a test file of sample data representing observed station pressures. Sample geostrophic wind fields calculated using these gridded surface pressures are presented in Figures 9 and 10. The adjusted wind fields are shown in Figures 11 and 12.

A forward trajectory calculated from the adjusted wind fields and using an initial location of 42^{o}N, 84^{o}W, an initial starting date and time of 0 hours, May 23, 1982, time intervals of 6 hours and a maximum time of 24 hours is illustrated in Figure 13.

The complete trajectory software system cannot be described as being fully operational. Minor revisions to the computer code are necessary for executions of the system of programs to be run using real station data. However, it is not recommended that these sample runs be done on the UNIVAC computer because of the prohibitive costs that would be involved. For this reason the software has been transferred to the Atmospheric Research Section's HP1000 minicomputer where no processing charges would be incurred. In order to complete the trajectory software system and have it operational on the HP1000 minicomputer, it is necessary to:

- make minor code modifications to the programs so that they are executable on the HP1000,
- make code revisions for sample executions using real data,
- test the complete software package using several sets of real data,
- document the complete software package.

GRIDDED SURFACE PRESSURE DATA

Date: 19820523
Hour: 0

10100	10130	10160	10190	10220
10160	10130	10160	10190	10220
10100	10130	10160	10190	10220
10100	10130	10160	10190	10220
10100	10130	10160	10190	10220

Date: 19820523
Hour: 6

				10220
10220	10220	10220	10220	10190
10190	10190	10190	10190	10160
10160	10160	10160	10160	10130
10130	10130	10130	10130	10100
10100	10100	10100	10100	

Date: 19820523
Hour: 18

10100	10100	10100	10100	10100
10130	10130	10130	10130	10130
10160	10160	10160	10160	10160
10190	10190	10190	10190	10190
10220	10220	10220	10220	10220

Date: 19820523
Hour: 12

				10100
10220	10190	10160	10130	10100
10220	10190	10160	10130	10100
10220	10190	10160	10130	10100
10220	10190	10160	10130	10100
10220	10190	10160	10130	

FIGURE 8

84-357

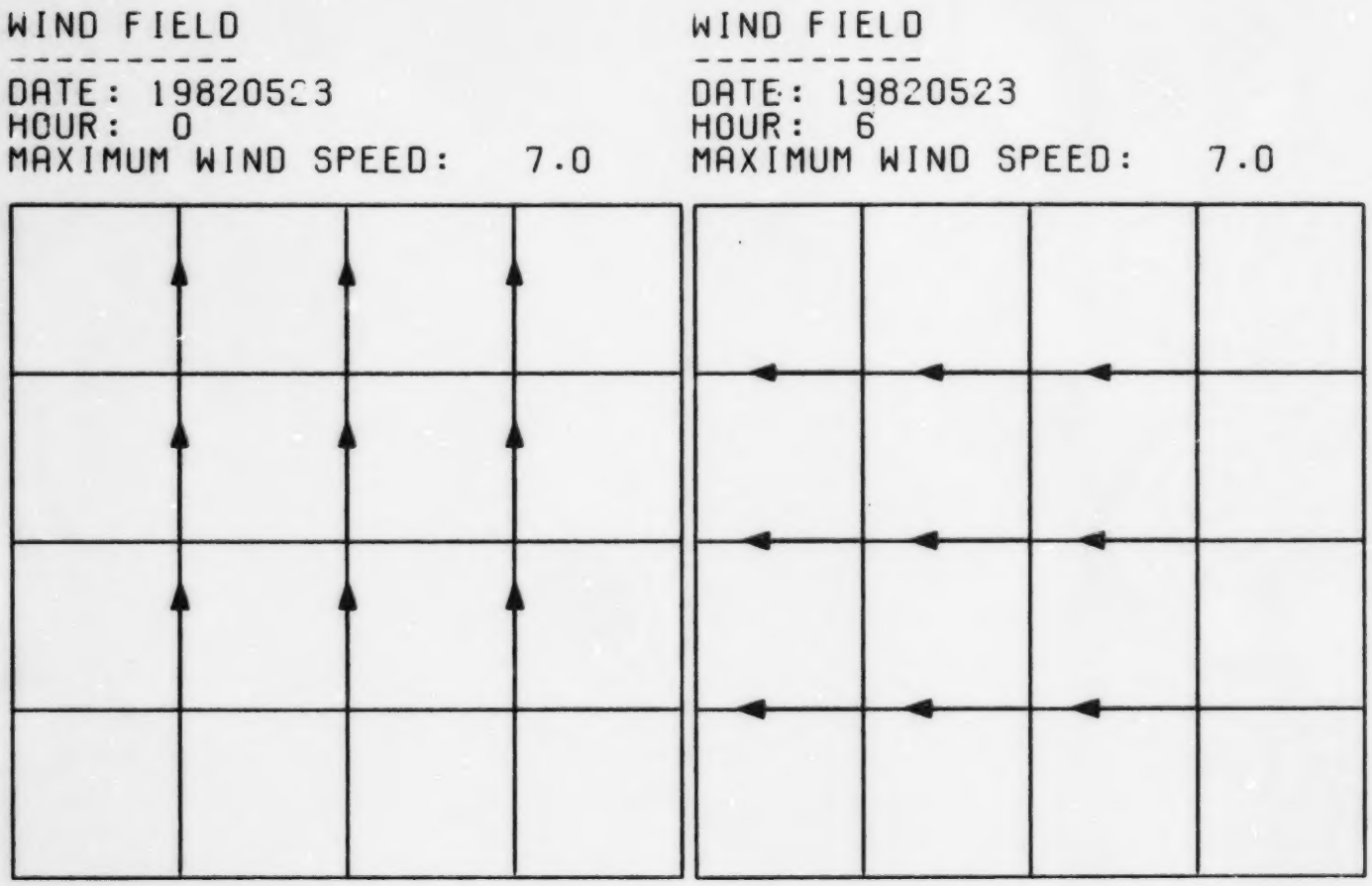
WIND FIELD
DATE: 19820523
HOUR: 0
MAXIMUM WIND SPEED: 7.0
WIND FIELD
DATE: 19820523
HOUR: 6
MAXIMUM WIND SPEED: 7.0

FIGURE 9

GEOSTROPHIC WIND FIELDS

WIND FIELD

DATE: 19820523
HOUR: 12
MAXIMUM WIND SPEED: 7.0

WIND FIELD

DATE: 19820523
HOUR: 18
MAXIMUM WIND SPEED: 7.0

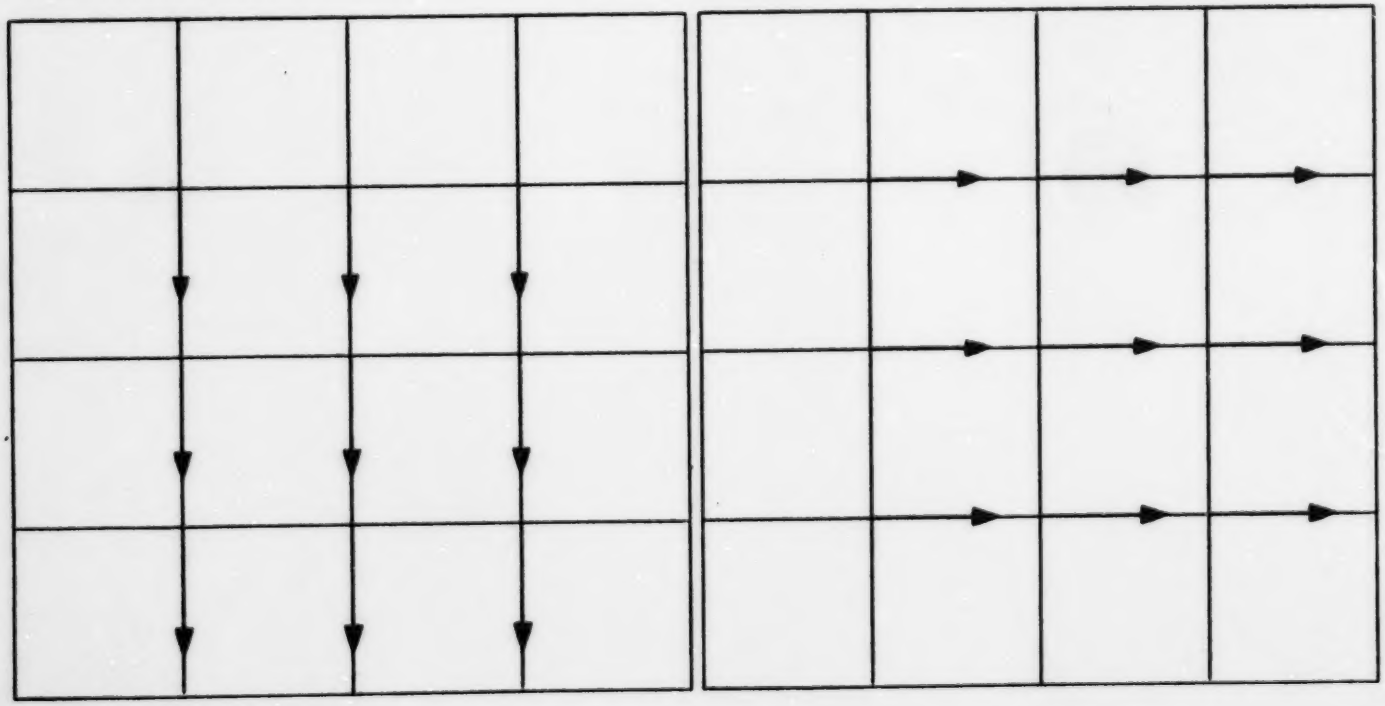

FIGURE 10

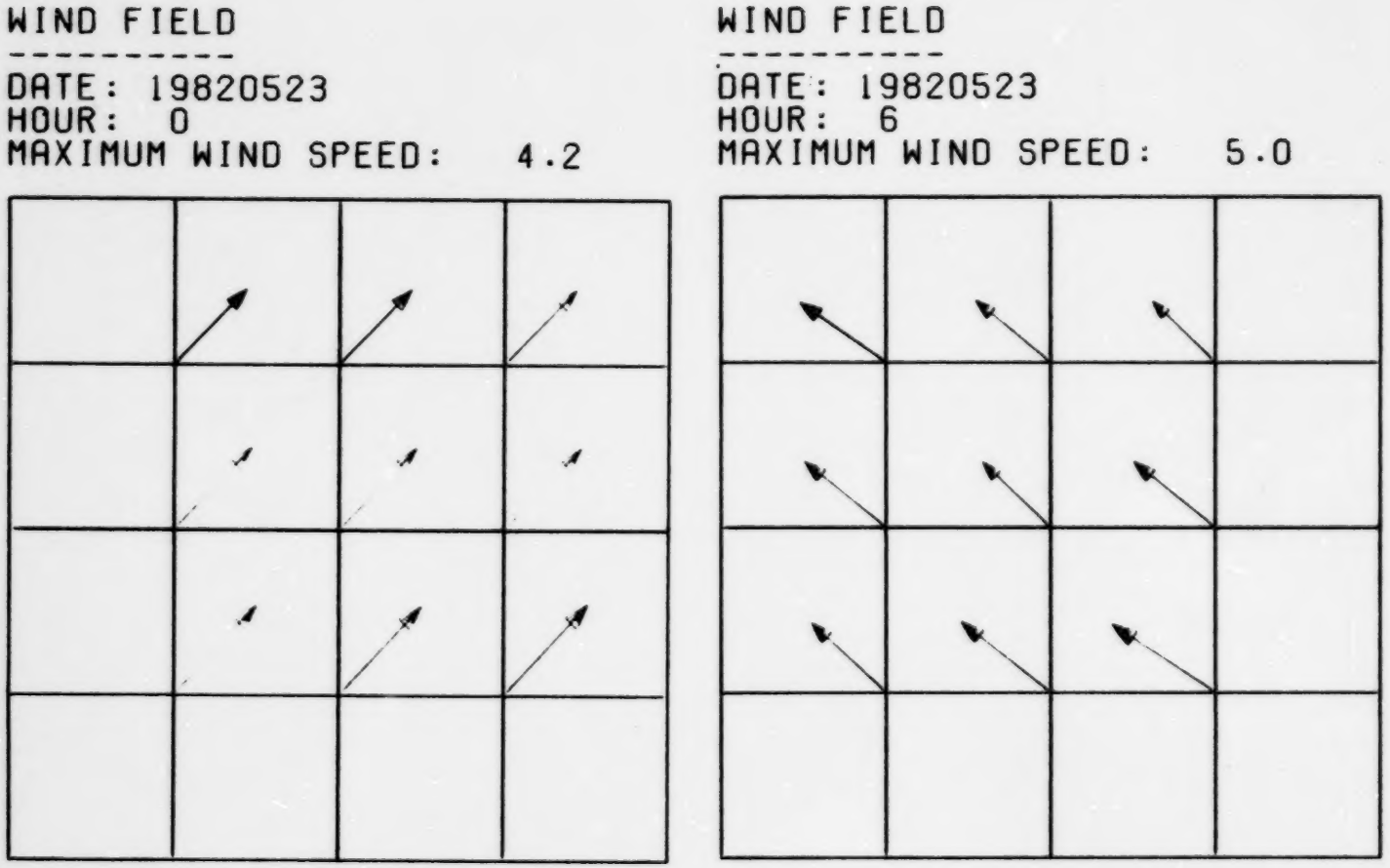
WIND FIELD
DATE: 19820523
HOUR: 0
MAXIMUM WIND SPEED: 4.2
WIND FIELD
DATE: 19820523
HOUR: 6
MAXIMUM WIND SPEED: 5.0

FIGURE 11

ADJUSTED WIND FIELDS

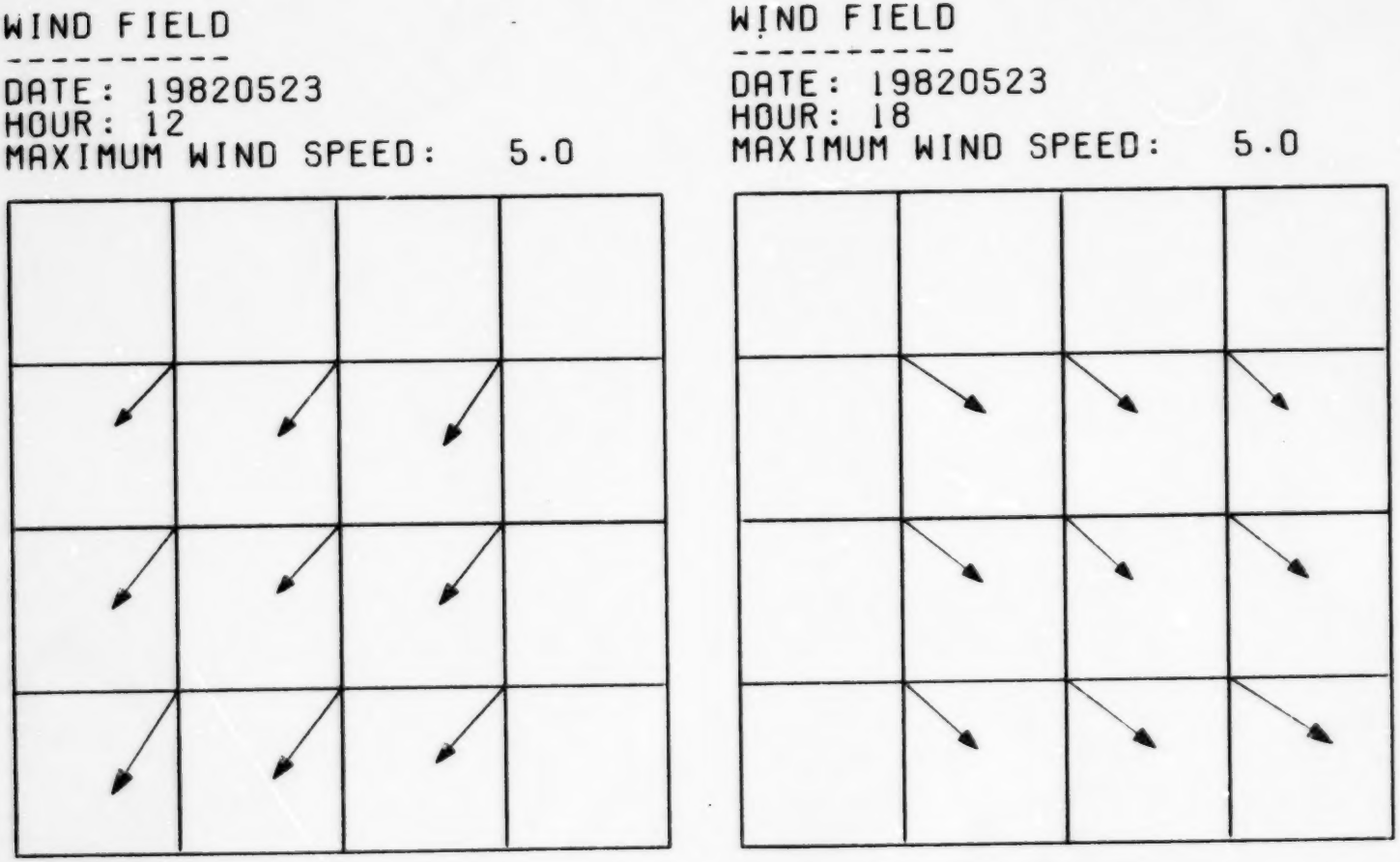

FIGURE 12

FORWARD TRAJECTORY

DATE 1982052?
MOON 0

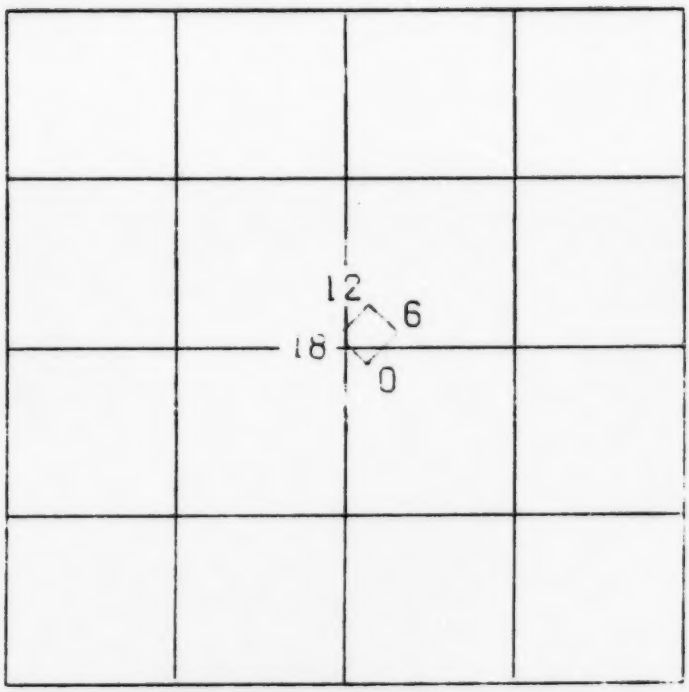

FIGURE 13

At the moment there are no firm plans to proceed with this additional work.

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